Full wwPDB X-ray Structure Validation Report (i)

Sep 13, 2023 – 05:01 AM EDT

PDB ID	:	4R0V
Title	:	[FeFe]-hydrogenase Oxygen Inactivation is Initiated by the Modification and Degradation of the H cluster 2Fe Subcluster
Authors	:	Swanson, S.D.; Ratzloff, M.W.; Mulder, D.W.; Artz, J.H.; Ghose, S.; Hoffman, A.; White, S.; Zadvornyy, O.A.; Broderick, J.B.; Bothner, B.; King, P.W.; Peters, J.W.
Deposited on	:	2014-08-01
Resolution	:	2.29 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

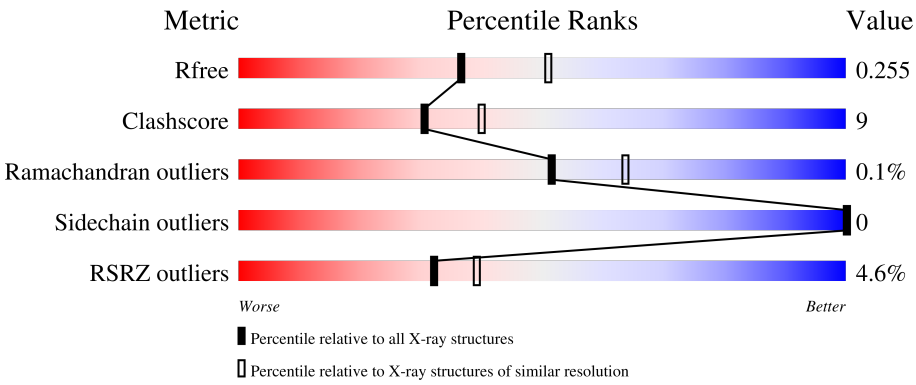
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	5% 70% 10% • 18%
1	B	514	3% 69% 10% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ARS	A	604	-	-	X	-
4	ARS	B	604	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6615 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fe-hydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3179	1998	550	606	25	0	2	0
1	B	410	3121	1963	539	594	25	0	2	0

There are 34 discrepancies between the modelled and reference sequences:

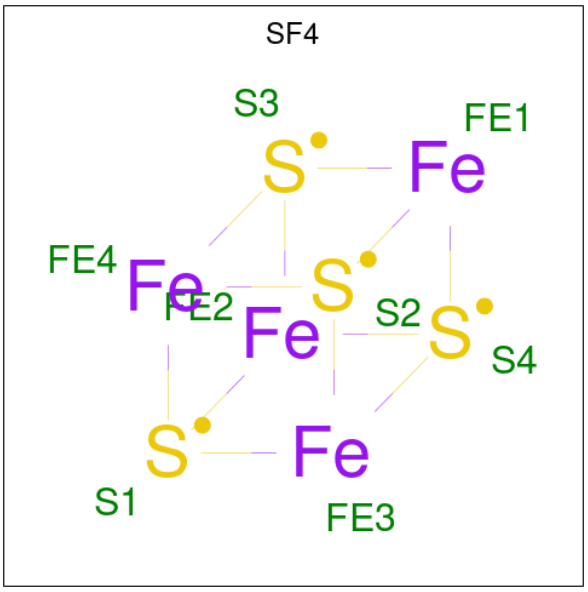
Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP Q9FYU1
A	499	GLU	-	expression tag	UNP Q9FYU1
A	500	ILE	-	expression tag	UNP Q9FYU1
A	501	GLU	-	expression tag	UNP Q9FYU1
A	502	GLY	-	expression tag	UNP Q9FYU1
A	503	ARG	-	expression tag	UNP Q9FYU1
A	504	GLN	-	expression tag	UNP Q9FYU1
A	505	LEU	-	expression tag	UNP Q9FYU1
A	506	GLY	-	expression tag	UNP Q9FYU1
A	507	TRP	-	expression tag	UNP Q9FYU1
A	508	SER	-	expression tag	UNP Q9FYU1
A	509	HIS	-	expression tag	UNP Q9FYU1
A	510	PRO	-	expression tag	UNP Q9FYU1
A	511	GLN	-	expression tag	UNP Q9FYU1
A	512	PHE	-	expression tag	UNP Q9FYU1
A	513	GLU	-	expression tag	UNP Q9FYU1
A	514	LYS	-	expression tag	UNP Q9FYU1
B	498	LEU	-	expression tag	UNP Q9FYU1
B	499	GLU	-	expression tag	UNP Q9FYU1
B	500	ILE	-	expression tag	UNP Q9FYU1
B	501	GLU	-	expression tag	UNP Q9FYU1
B	502	GLY	-	expression tag	UNP Q9FYU1
B	503	ARG	-	expression tag	UNP Q9FYU1
B	504	GLN	-	expression tag	UNP Q9FYU1
B	505	LEU	-	expression tag	UNP Q9FYU1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	GLY	-	expression tag	UNP Q9FYU1
B	507	TRP	-	expression tag	UNP Q9FYU1
B	508	SER	-	expression tag	UNP Q9FYU1
B	509	HIS	-	expression tag	UNP Q9FYU1
B	510	PRO	-	expression tag	UNP Q9FYU1
B	511	GLN	-	expression tag	UNP Q9FYU1
B	512	PHE	-	expression tag	UNP Q9FYU1
B	513	GLU	-	expression tag	UNP Q9FYU1
B	514	LYS	-	expression tag	UNP Q9FYU1

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0
2	B	1	8	4	4	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	2	2	2	0	0
3	B	2	2	2	0	0

- Molecule 4 is ARSENIC (three-letter code: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	As		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

- Molecule 5 is water.

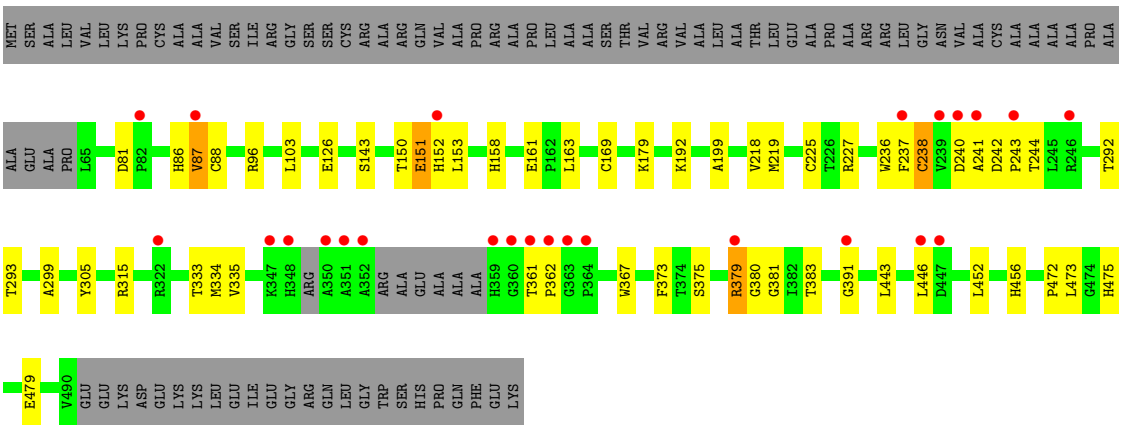
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	147	147	147	0	0
5	B	146	146	146	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

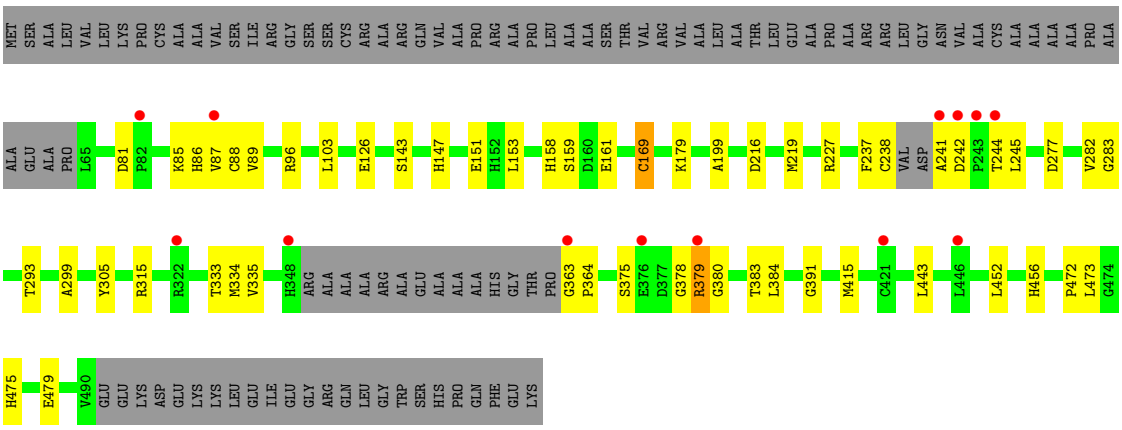
- Molecule 1: Fe-hydrogenase

Chain A:



- Molecule 1: Fe-hydrogenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.64Å 70.96Å 94.69Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	35.00 – 2.29 39.37 – 2.29	Depositor EDS
% Data completeness (in resolution range)	88.2 (35.00-2.29) 88.2 (39.37-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.252 0.217 , 0.255	Depositor DCC
R_{free} test set	2098 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6615	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0524e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ARS, SF4, CSD, CL, CSO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.90	2/3220 (0.1%)	0.97	8/4357 (0.2%)
1	B	0.89	1/3161 (0.0%)	1.01	7/4276 (0.2%)
All	All	0.90	3/6381 (0.0%)	0.99	15/8633 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	VAL	C-N	-5.28	1.22	1.34
1	A	88	CSD	C-N	5.22	1.46	1.34
1	A	150	THR	C-N	5.21	1.46	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	88	CSD	O-C-N	-18.11	93.73	122.70
1	B	88	CSD	CA-C-N	13.65	147.24	117.20
1	A	88	CSD	O-C-N	-11.19	104.79	122.70
1	B	88	CSD	C-N-CA	11.09	149.42	121.70
1	A	151	GLU	O-C-N	-7.77	110.26	122.70
1	A	88	CSD	CA-C-N	7.62	133.95	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	380	GLY	N-CA-C	-7.32	94.79	113.10
1	B	379	ARG	CB-CA-C	6.82	124.04	110.40
1	A	380	GLY	N-CA-C	-6.61	96.57	113.10
1	A	379	ARG	CB-CA-C	6.28	122.96	110.40
1	B	379	ARG	N-CA-C	-5.90	95.07	111.00
1	A	379	ARG	N-CA-C	-5.65	95.74	111.00
1	A	151	GLU	CA-C-N	5.26	128.78	117.20
1	A	81	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	81	ASP	CB-CG-OD1	5.15	122.94	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	CSO	Mainchain
1	A	87	VAL	Mainchain
1	B	169[A]	CSO	Mainchain
1	B	169[B]	CSO	Mainchain
1	B	237	PHE	Mainchain
1	B	87	VAL	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3179	0	3162	61	0
1	B	3121	0	3108	62	0
2	A	8	0	0	1	0
2	B	8	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	8	0
4	B	1	0	0	9	0
5	A	147	0	0	5	0
5	B	146	0	0	5	0
All	All	6615	0	6270	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:THR:CG2	1:A:362:PRO:HD2	1.51	1.41
1:A:361:THR:HG23	1:A:362:PRO:CD	1.52	1.38
1:A:475:HIS:NE2	4:B:604:ARS:AS	2.40	1.14
4:A:604:ARS:AS	1:B:475:HIS:NE2	2.40	1.14
1:A:292:THR:HB	5:A:829:HOH:O	1.46	1.14
1:A:87:VAL:HG22	1:A:218:VAL:HB	1.19	1.13
1:A:158:HIS:CG	4:A:604:ARS:AS	2.66	1.08
1:A:333:THR:HG22	1:A:383:THR:CG2	1.86	1.04
1:B:333:THR:HG22	1:B:383:THR:CG2	1.87	1.04
1:A:362:PRO:HG3	1:B:241:ALA:HB3	1.43	1.00
1:A:158:HIS:ND1	4:A:604:ARS:AS	2.57	0.98
1:B:151:GLU:OE2	4:B:604:ARS:AS	2.42	0.97
1:A:192:LYS:HE2	1:A:237:PHE:CE1	2.01	0.96
1:B:151:GLU:CD	4:B:604:ARS:AS	2.65	0.95
1:B:161:GLU:OE1	4:B:604:ARS:AS	2.46	0.94
1:A:158:HIS:HB2	4:A:604:ARS:AS	2.29	0.92
1:A:333:THR:HG22	1:A:383:THR:HG22	1.52	0.91
1:B:333:THR:HG22	1:B:383:THR:HG22	1.51	0.89
1:B:158:HIS:ND1	4:B:604:ARS:AS	2.67	0.87
1:A:361:THR:CG2	1:A:362:PRO:CD	2.30	0.86
1:B:151:GLU:OE1	4:B:604:ARS:AS	2.54	0.86
1:A:362:PRO:CG	1:B:241:ALA:HB3	2.07	0.85
1:B:169[B]:CSO:SG	1:B:415[B]:MET:CE	2.66	0.84
1:A:158:HIS:CB	4:A:604:ARS:AS	2.85	0.84
1:A:151:GLU:OE2	4:A:604:ARS:AS	2.56	0.82
1:A:152:HIS:HD2	1:A:367:TRP:CE3	1.97	0.81
1:B:244:THR:HG23	1:B:245:LEU:N	1.96	0.80
1:B:143:SER:HB2	1:B:473:LEU:HD13	1.62	0.80
1:A:143:SER:HB2	1:A:473:LEU:HD13	1.63	0.80
1:B:333:THR:HA	1:B:383:THR:HG22	1.66	0.77
1:A:161:GLU:OE1	4:A:604:ARS:AS	2.63	0.77
1:A:333:THR:HA	1:A:383:THR:HG22	1.65	0.77
1:B:333:THR:HG22	1:B:383:THR:HG21	1.68	0.76
1:A:333:THR:HG22	1:A:383:THR:HG21	1.67	0.75
1:B:169[B]:CSO:SG	1:B:415[B]:MET:HE1	2.26	0.75
1:A:192:LYS:HE2	1:A:237:PHE:HE1	1.52	0.74
1:A:335:VAL:HG11	1:A:379:ARG:NH2	2.02	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HG11	1:B:379:ARG:NH2	2.01	0.73
1:A:152:HIS:CD2	1:A:367:TRP:CE3	2.79	0.70
1:A:87:VAL:CG2	1:A:218:VAL:HB	2.12	0.70
1:B:244:THR:HG23	1:B:245:LEU:H	1.56	0.69
1:A:333:THR:CG2	1:A:383:THR:HG22	2.22	0.69
1:B:333:THR:CG2	1:B:383:THR:HG22	2.23	0.69
1:B:169[B]:CSO:SG	1:B:415[B]:MET:HE3	2.33	0.68
1:B:147:HIS:NE2	4:B:604:ARS:AS	2.87	0.68
4:A:604:ARS:AS	1:B:475:HIS:CE1	3.08	0.66
1:A:143:SER:HB2	1:A:473:LEU:CD1	2.26	0.65
1:B:143:SER:HB2	1:B:473:LEU:CD1	2.25	0.65
1:B:305:TYR:HA	1:B:334:MET:HE3	1.80	0.65
1:B:244:THR:CG2	1:B:245:LEU:H	2.11	0.63
1:A:333:THR:CG2	1:A:383:THR:CG2	2.73	0.63
1:B:244:THR:CG2	1:B:245:LEU:N	2.61	0.63
1:A:361:THR:CG2	1:A:362:PRO:N	2.62	0.61
1:A:362:PRO:CG	1:B:241:ALA:CB	2.78	0.60
1:B:147:HIS:CE1	1:B:151:GLU:OE2	2.53	0.60
1:B:158:HIS:CG	4:B:604:ARS:AS	3.15	0.60
1:B:375:SER:OG	1:B:379:ARG:HB2	2.02	0.59
1:A:96:ARG:NH2	1:A:443:LEU:O	2.30	0.59
1:A:227:ARG:HD3	5:A:790:HOH:O	2.02	0.58
1:B:227:ARG:HD3	5:B:787:HOH:O	2.03	0.58
1:B:333:THR:CG2	1:B:383:THR:CG2	2.75	0.56
1:A:236:TRP:C	1:A:238:CSO:N	2.59	0.55
1:A:86:HIS:HE1	1:A:126:GLU:OE1	1.90	0.55
1:A:373:PHE:CZ	1:A:381:GLY:HA3	2.42	0.54
1:B:238:CSO:CB	1:B:245:LEU:O	2.55	0.54
1:A:86:HIS:CE1	1:A:126:GLU:OE1	2.60	0.54
1:A:375:SER:OG	1:A:379:ARG:HB2	2.07	0.54
1:A:362:PRO:HG2	1:B:241:ALA:CB	2.38	0.53
1:B:86:HIS:CE1	1:B:126:GLU:OE1	2.62	0.52
1:B:96:ARG:NH2	1:B:443:LEU:O	2.32	0.51
1:A:241:ALA:HB2	1:B:159:SER:HB2	1.93	0.51
1:A:240:ASP:O	1:A:241:ALA:HB3	2.11	0.51
1:A:158:HIS:CD2	1:B:479:GLU:HG3	2.46	0.51
1:B:179:LYS:HD2	5:B:822:HOH:O	2.10	0.50
1:B:147:HIS:NE2	1:B:151:GLU:OE2	2.44	0.50
1:A:199:ALA:HA	1:A:219:MET:CE	2.43	0.49
1:A:179:LYS:HD2	5:A:815:HOH:O	2.12	0.49
1:B:85:LYS:HD2	1:B:216:ASP:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASP:O	1:B:242:ASP:OD1	2.29	0.49
1:A:315:ARG:HD3	1:A:452:LEU:HD13	1.96	0.48
1:B:199:ALA:HA	1:B:219:MET:CE	2.43	0.48
1:A:479:GLU:HG3	1:B:158:HIS:CD2	2.49	0.47
1:A:305:TYR:HA	1:A:334:MET:HE3	1.95	0.47
1:B:315:ARG:HD3	1:B:452:LEU:HD13	1.96	0.47
1:B:472:PRO:O	1:B:473:LEU:HB2	2.14	0.47
1:B:305:TYR:HA	1:B:334:MET:CE	2.44	0.47
1:A:305:TYR:HA	1:A:334:MET:CE	2.45	0.47
1:A:472:PRO:O	1:A:473:LEU:HB2	2.15	0.46
1:A:456:HIS:HD2	5:A:807:HOH:O	1.99	0.45
1:A:361:THR:HG22	1:A:362:PRO:N	2.30	0.45
1:B:86:HIS:HE1	1:B:126:GLU:OE1	1.99	0.45
1:B:456:HIS:HD2	5:B:809:HOH:O	1.99	0.45
1:B:158:HIS:HB2	4:B:604:ARS:AS	2.77	0.45
1:A:333:THR:CA	1:A:383:THR:HG22	2.41	0.44
1:A:375:SER:OG	1:A:379:ARG:N	2.50	0.44
1:B:282:VAL:HG22	1:B:283:GLY:N	2.32	0.44
1:B:103:LEU:HD21	5:B:797:HOH:O	2.17	0.43
1:A:242:ASP:C	1:A:244:THR:H	2.21	0.43
1:B:238:CSO:CA	1:B:245:LEU:O	2.66	0.43
1:B:126:GLU:HA	1:B:277:ASP:OD2	2.19	0.43
1:B:378:GLY:O	1:B:379:ARG:C	2.57	0.42
1:A:238:CSO:HB2	1:A:243:PRO:HA	2.01	0.42
1:B:363:GLY:O	1:B:364:PRO:C	2.57	0.42
1:A:293:THR:HB	1:A:299:ALA:HB2	2.01	0.42
1:A:152:HIS:CG	1:A:163:LEU:HD12	2.55	0.41
1:B:415[B]:MET:CE	5:B:727:HOH:O	2.67	0.41
1:B:153:LEU:HD23	1:B:153:LEU:HA	1.89	0.41
1:A:152:HIS:CE1	1:A:163:LEU:HG	2.56	0.41
1:B:293:THR:HB	1:B:299:ALA:HB2	2.02	0.41
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.86	0.41
1:B:384:LEU:HD12	1:B:384:LEU:HA	1.94	0.41
1:A:225:CYS:HB2	2:A:601:SF4:S3	2.61	0.40
1:A:103:LEU:HD21	5:A:799:HOH:O	2.22	0.40
1:B:333:THR:CA	1:B:383:THR:HG22	2.43	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/514 (80%)	401 (98%)	9 (2%)	1 (0%)	47	58
1	B	403/514 (78%)	392 (97%)	11 (3%)	0	100	100
All	All	814/1028 (79%)	793 (97%)	20 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/399 (84%)	333 (100%)	0	100	100
1	B	328/399 (82%)	328 (100%)	0	100	100
All	All	661/798 (83%)	661 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	152	HIS
1	A	195	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	440	GLN
1	B	86	HIS
1	B	195	GLN
1	B	440	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSO	B	169[B]	-	3,6,7	0.80	0	0,6,8	-	-
1	CSO	A	169[A]	-	3,6,7	1.10	0	0,6,8	-	-
1	CSD	B	88	1	3,7,8	1.44	0	1,8,10	3.08	1 (100%)
1	CSO	B	238	1	3,6,7	0.97	0	0,6,8	-	-
1	CSD	A	88	1	3,7,8	1.52	0	1,8,10	3.59	1 (100%)
1	CSO	A	169[B]	-	3,6,7	1.91	1 (33%)	0,6,8	-	-
1	CSO	B	169[A]	-	3,6,7	0.96	0	0,6,8	-	-
1	CSO	A	238	1	3,6,7	0.97	0	0,6,8	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	B	169[B]	-	-	0/1/5/7	-
1	CSO	A	169[A]	-	-	0/1/5/7	-
1	CSD	B	88	1	-	1/2/6/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	B	238	1	-	1/1/5/7	-
1	CSD	A	88	1	-	1/2/6/8	-
1	CSO	A	169[B]	-	-	1/1/5/7	-
1	CSO	B	169[A]	-	-	1/1/5/7	-
1	CSO	A	238	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169[B]	CSO	CB-CA	2.79	1.60	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	CSD	OD1-SG-CB	3.59	112.37	105.54
1	B	88	CSD	OD1-SG-CB	3.08	111.40	105.54

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	88	CSD	CA-CB-SG-OD1
1	A	169[B]	CSO	N-CA-CB-SG
1	B	88	CSD	CA-CB-SG-OD1
1	B	238	CSO	N-CA-CB-SG
1	B	169[A]	CSO	N-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	169[B]	CSO	3	0
1	B	238	CSO	2	0
1	A	238	CSO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SF4	B	601	1	0,12,12	-	-	-		
2	SF4	A	601	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	601	1	-	-	0/6/5/5
2	SF4	A	601	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SF4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	87:VAL	C	88:CSD	N	1.61

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	416/514 (80%)	0.05	25 (6%)	21	28	30, 45, 83, 153	2 (0%)
1	B	407/514 (79%)	-0.11	13 (3%)	47	54	30, 44, 78, 123	2 (0%)
All	All	823/1028 (80%)	-0.03	38 (4%)	32	39	30, 44, 80, 153	4 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	HIS	10.6
1	A	241	ALA	9.4
1	A	240	ASP	8.0
1	A	360	GLY	7.5
1	A	361	THR	6.4
1	A	362	PRO	6.3
1	A	352	ALA	5.6
1	A	237	PHE	5.5
1	B	241	ALA	5.3
1	A	87	VAL	5.2
1	B	376	GLU	4.8
1	A	350	ALA	4.6
1	A	351	ALA	4.3
1	A	246	ARG	4.3
1	B	242	ASP	3.9
1	A	391	GLY	3.9
1	B	244	THR	3.8
1	B	446	LEU	3.3
1	B	322	ARG	3.3
1	A	152	HIS	3.1
1	A	239	VAL	3.0
1	A	322	ARG	3.0
1	B	348	HIS	3.0
1	A	348	HIS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	446	LEU	2.8
1	A	363	GLY	2.7
1	B	82	PRO	2.6
1	A	243	PRO	2.5
1	B	363	GLY	2.4
1	B	243	PRO	2.4
1	A	82	PRO	2.3
1	B	421	CYS	2.3
1	A	379	ARG	2.2
1	B	87	VAL	2.2
1	A	347	LYS	2.2
1	A	447	ASP	2.1
1	B	379	ARG	2.1
1	A	364	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	A	238	7/8	0.60	0.38	45,52,59,60	0
1	CSO	B	238	7/8	0.64	0.34	45,52,59,60	0
1	CSO	B	169[B]	7/8	0.75	0.23	22,33,35,38	4
1	CSO	B	169[A]	7/8	0.75	0.23	32,33,38,47	4
1	CSO	A	169[A]	7/8	0.83	0.24	30,34,38,43	4
1	CSO	A	169[B]	7/8	0.83	0.24	25,35,36,47	4
1	CSD	B	88	8/9	0.89	0.14	30,36,44,49	3
1	CSD	A	88	8/9	0.89	0.18	31,35,43,48	3

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ARS	A	604	1/1	0.56	0.37	69,69,69,69	0
2	SF4	A	601	8/8	0.63	0.18	24,27,40,41	0
2	SF4	B	601	8/8	0.83	0.10	24,27,40,41	0
4	ARS	B	604	1/1	0.89	0.10	71,71,71,71	0
3	CL	A	602	1/1	0.97	0.10	73,73,73,73	0
3	CL	B	603	1/1	0.99	0.12	78,78,78,78	0
3	CL	A	603	1/1	0.99	0.23	40,40,40,40	0
3	CL	B	602	1/1	0.99	0.21	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.